November 1, 1971

FRA-TM-22

BUCKLING IN FAST REACTORS. I.

B. I. Spinrad

Argonne National Laboratory
Applied Physics Division
9700 South Cass Avenue
Argonne, Illinois 60439

FRA TECHNICAL MEMORANDUM NO. 22

Results reported in the FRA-TM series of memoranda frequently are preliminary and subject to revision. Consequently they should not be quoted or referenced without the author's permission.

Work performed under the auspices of the U. S. Atomic Energy Commission.

Buckling in Fast Reactors. I.

B. I. SPINRAD

Applied Physics Division
Argonne National Laboratory
Argonne, Illinois 60439

ABSTRACT

The energy-dependent reactor diffusion equation can be expanded in a series of products of purely spectral and purely spatial components. A convenient set of base spectra are the coefficients when the fundamental mode spectrum is expressed as a power series in B^2. The algorithm for forming these spectra is relatively simple. Some of the properties of these spectra are exhibited, and the reduction of the reactor problem to one of definable overlapping diffusion groups is explored.

INTRODUCTION

The concept of buckling was introduced in the first explorations of reactors for several reasons:

(1) The reactors were large and almost all of their volume was describable by the fundamental spatial and spectral mode.

(2) Reflector savings were relatively small, and the buckling provided an accurate estimate of critical dimensions.

(3) With infinite multiplication only slightly greater than unity, measurement of buckling, combined with estimation of the form of P(B) — from experiment or theory — permitted more accurate determination of k_∞ than any other technique.

The first reactors were large, natural-uranium-fueled ones, to which these comments are very pertinent. However, the early fast reactors were small, highly reflected, and with k_∞ in the core around 2. To such reactors, the concept of buckling was not useful, and the main theoretical approaches emphasize transport and multigroup calculations, with the fundamental mode only one of many important spatial modes in the reactor.

However, the relative simplicity of buckling measurements prompted experimental groups, first at Los Alamos and then at Argonne[1] to attempt to determine buckling and bring its measurements into consonance with the theoretical models available. A particularly large effort was expended in determining the (negative) buckling of an assembly of natural uranium.[2]

As the design of fast reactors for central-station power generation evolved, it became apparent that these reactors were reverting toward systems for which the buckling could again be a useful parameter. The

incorporation of large amounts of ^{238}U into the core to facilitate internal breeding brought values of k_∞ into the range 1.0-1.5. Even at the high power densities of breeders, the size of reactor cores to supply heat for 1000 MW of electrical generation becomes large enough so that we expect major portions of the core to be only mildly influenced by reflector transients. With understanding of the behavior of reflector savings, the estimation or measurement of buckling then becomes a useful predictor of criticality in fast reactors. Thus, Hummel was able, through the ELMOE code,[3] to use changes in buckling of reactors to separate reactivity effects which are intrinsic in the core from those which are reflector-induced. In France, there have been a number of experiments on buckling, both to determine core critical properties and to use buckling as a measure of reactivity difference in substitution experiments.[4]

Up to now, the interpretation of buckling experiments has been primarily a matter of comparing measured values with those deduced from such basic calculations as ELMOE. Where discrepancies appear, the cross-section set itself must bear the burden. This is entirely proper in the ultimate; however, the discovery of adjustments to nuclear data is much eased if a simpler interpretation of buckling can lead to another, easily characterized integral parameter. In thermal reactors, as had been mentioned, this interpretation is provided by the relation

$$k_\infty P(B) = 1, \qquad (1)$$

where $P(B)$ is the nonleakage probability associated with buckling B^2. Equation (1) holds for critical systems, which is a strong experimental condition. In thermal reactors, $P(B)$ is at least partly measurable, since it is related to migration during slowing down, which is measurable

and only slightly perturbed by absorption, and to thermal neutron migration which is either accurately described by diffusion theory in the global sense, or is small. The standard interpretation of P(B) is as the Fourier transform of the spatial distribution of flux leading to absorption, from a point source of fission neutrons in an infinite medium whose slowing-down and absorption characteristics are identical with those of the reactor, but in which fission does not occur (Weinberg[5]).

This (correct) interpretation has discouraged attempts to estimate P(B) for fast reactors. It is well-nigh impossible to mock up a fast reactor core for migration measurements, and simultaneously to suppress fission. Thus, estimation of P(B) is limited to the examination of the variation of B^2 with, for example, ν, in ELMOE-type codes. This procedure is again correct; however, it suffers from the fact that inference of P(B) for negative or complex B^2, which is often desirable to estimate reflector-induced transients, is a very imprecise extrapolation.

The first portion of this paper is the presentation of a method for deriving P(B) as a power series in B^2, using purely spectral calculations. The significance of this technique lies not only in its ability to explore P(B) for negative or complex B^2, but also in the fact that the spectra associated with powers of B^2 have in themselves interesting properties which suggest the utility of overlapping multigroup formalisms and Lie series for calculating global properties of fast reactors.

A POWER SERIES FOR P(B)

Assuming diffusion theory, the space-energy equations for any reactor may be written as:

$$-D(E)\nabla^2\phi(\vec{r},E) + \left[\Sigma_a(E) + \Sigma_s(E)\right]\phi(\vec{r},E) - \int_E^\infty \Sigma_s(E')\phi(\vec{r},E')P_s(E' \to E)\, dE'$$

$$= \chi(E) \int_0^\infty \nu\Sigma_f(E')\phi(\vec{r},E')\, dE' \,. \qquad (2)$$

The symbols in Eq. (2) have their canonical meanings. The only unusual ones are $P_s(E' \to E)$, the probability that a scattering event for a neutron of energy E' will lead to its emergence at energy E, and $\chi(E)$, the fission spectrum. If there are several fissionable isotopes, $\nu\Sigma_f$ is interpreted as $\sum_i \nu_i\Sigma_{fi}$ for the "i" isotopes. In addition to the assumptions of diffusion theory, Eq. (2) assumes that scattering is isotropic, which is virtually within diffusion theory, and that the fission spectrum is invariant to fissioning species. This latter assumption is almost correct if there is a dominant fissionable material, and is easily set right by defining a $\bar{\chi}$; it is made only to simplify notation.

Suppose there exists a fundamental mode and a critical reactor. Then the fundamental mode may be written

$$\phi_0(\vec{r},E) = f_0(\vec{r},B_0)S_0(E) \,, \qquad (3)$$

where

$$\nabla^2 f_0(\vec{r},B_0) = -B_0^2 f_0(\vec{r},B_0) \,. \qquad (4)$$

Substitution of Eqs. (3) and (4) into Eq. (2) permits factorization and division of f_0, and leads to

$$\left[B_0^2 D(E) + \Sigma_a(E) + \Sigma_s(E)\right]S_0(E) - \int_E^\infty \Sigma_s(E')S_0(E')P_s(E' \to E)\, dE'$$

$$= \chi(E) \int_0^\infty \nu\Sigma_f(E')S_0(E')\, dE' \,. \qquad (5)$$

If we integrate Eq. (5) over all E, remembering that $\chi(E)$ is normalized to unity and that the integral of P_s over emergent energies is also unity, we get:

$$\int_0^\infty \left[B_0^2 D(E) + \Sigma_a(E)\right] S_0(E)\, dE = \int_0^\infty \nu\Sigma_f(E')S_0(E')\, dE' . \tag{6}$$

Useful relations may also be derived for an idealized infinite-medium experiment. If an infinite medium has a unit fission-spectrum source per unit volume, then the spectrum of neutrons would be given by S_∞, where S_∞ is the spectrum which solves:

$$\left[\Sigma_a(E) + \Sigma_s(E)\right] S_\infty(E) - \int_E^\infty \Sigma_s(E')S_0(E')P_s(E' \to E)\, dE' = \chi(E) . \tag{7}$$

Integration over all energies reveals that since the neutron production rate, $\int \chi\, dE$, is unity, so is the absorption rate, $\int \Sigma_a S_\infty\, dE$. If we now ask what the production rate would be if the spectrum were permitted to cause fission, it would be $\int \nu\Sigma_f S_\infty\, dE$. Thus,

$$k_\infty = \int_0^\infty \nu\Sigma_f S_\infty\, dE . \tag{8}$$

The fact that systems with small bucklings have spectra approaching those of infinite media is well known. It suggests that we look for solutions of S_0 in the form of

$$S_0 = \sum_{n=0}^{\infty} (-B_0^2)^n G_n \tag{9}$$

with

$$G_0 = S_\infty . \tag{10}$$

Substitution of Eq. (9) into Eq. (5) yields:

$$\sum_{n=0}^{\infty} (-B_0^2)^n \left\{ \left[\Sigma_a(E) + \Sigma_s(E) \right] G_n(E) - \int_E^{\infty} \Sigma_s(E') G_n(E') P(E' \to E)\, dE \right.$$

$$\left. - \chi(E) \int_0^{\infty} \nu\Sigma_f(E') G_n(E')\, dE \right\} = \sum_{n=1}^{\infty} (-B_0^2)\, D(E) G_{n-1}(E) . \qquad (11)$$

We now define G_n by the relation

$$\left[\Sigma_a(E) + \Sigma_a(E) \right] G_{n+1}(E) - \int_E^{\infty} \Sigma_s(E') G_{n+1}(E') P_s(E' \to E)\, dE' = D(E) G_n(E) . \qquad (12)$$

Substituting Eq. (12) into Eq. (11) gives:

$$\left[\Sigma_a(E) + \Sigma_s(E) \right] G_0(E) - \int_E^{\infty} \Sigma_s(E') G_0(E') P_s(E' \to E)\, dE'$$

$$= \chi(E) \int_0^{\infty} \nu\Sigma_f(E') \sum_{n=0}^{\infty} (-B_0^2) G_n(E')\, dE' . \qquad (13)$$

Since $G_0 = S_\infty$, we may substitute Eq. (7) to get

$$1 = \sum_{n=0}^{\infty} (-B_0^2) \int_0^{\infty} \nu\Sigma_f(E') G_n(E')\, dE' . \qquad (14)$$

From Eq. (8), we next get

$$k_\infty \sum_{n=0}^{\infty} (-B_0^2)^n \left[\int_0^{\infty} \nu\Sigma_f(E') G_n(E')\, dE' \right] \Big/ \left[\int_0^{\infty} \nu\Sigma_f(E') G_0(E')\, dE' \right] = 1 . \qquad (15)$$

All that remains is to define

$$g_n = \int_0^\infty \nu\Sigma_f(E')G_n(E')\,dE' \Big/ \int_0^\infty \nu\Sigma_f(E')G_0(E')\,dE' , \tag{16}$$

and to identify Eq. (15) with Eq. (1). This yields

$$P(B) = \sum_{n=0}^{\infty} g_n(-B^2)^n . \tag{17}$$

(See footnote a.)

The above proof suggests an algorithm for computing G_n and g_n. We take as given a program which will solve for the infinite medium spectrum with a fission spectrum source. That is, we assume that we have means of solving Eq. (7); a subroutine of ELMOE will do as an example. Then, the G_n may be computed by successive substitution of $D\,G_{n-1}$ for χ, and the g_n by direct quadrature. The result is a purely spectral calculation of P(B).

EXAMPLE: AN AGING SYSTEM

We may illustrate the process analytically by taking as an illustration a system with the following properties:

(a) monoenergetic fission source at energy E_0, lethargy 0;

(b) slowing-down in a continuous mode without absorption to lethargy U; and

(c) absorption and fission without further migration on reaching lethargy U.

These assumptions mean that Eq. (5) may be written as

$$B_0^2 D\,S_0 + \frac{\partial}{\partial u}\left[\xi\Sigma_s S_0\right] = k_\infty \delta(u)\left[\xi\Sigma_s S_0\right]_U , \tag{18}$$

$$\delta_n = \int_0^\infty \nu\Sigma_f(E')\phi_0(E')\,dE' \Big/ \int_0^\infty \nu\Sigma_f(E')\phi_n(E')\,dE' \,. \qquad (26)$$

and to identify $\mathrm{Eq.}\ (18)$ with $\mathrm{Eq.}\ (1)$. This yields

$$P(B) = \sum_{n=0}^{\infty} \xi_n (-B^2)^n \,. \qquad (27)$$

(See footnote 4.)

The above proof suggests an algorithm for computing δ_n and ξ_n. We take as given a program which will solve for the infinite medium spectrum with a fission spectrum source. That is, we assume that we have means of solving Eq. (7); a subroutine of ENDF VIII do as an example. Then, the ξ_n may be computed by successive substitution of ϕ_{n-1} for χ, and the ξ_n by direct quadrature. The result is a purely spectral calculation of P(B).

EXAMPLE: AN ASYMPTOTIC SYSTEM

We may illustrate the process analytically by taking as an illustration a system with the following properties:

(a) monoenergetic fission source at energy E_0, lethargy U_0

(b) slowing-down in a continuous mode without absorption to lethargy U; and

(c) absorption and fission without further migration or reaching lethargy U.

These assumptions mean that Eq. (5) may be written as

$$\mathrm{Eq.}\ (18)$$

where we have converted to lethargy space, and need only consider u in (0,U). Equation (7) becomes

$$\frac{\partial}{\partial u}\left[\xi\Sigma\, S_\infty\right] = \delta(u) . \tag{19}$$

Then,

$$\left.\begin{aligned} G_0 &= \frac{1}{\xi\Sigma_s} , \\ G_1 &= \frac{1}{\xi\Sigma}\int_0^u \frac{D\, du'}{\xi\Sigma_s(u')} , \\ G_2 &= \frac{1}{\xi\Sigma_s}\int_0^u \frac{D}{\xi\Sigma_s}(u')\, dU' \int_0^{u'} \frac{D}{\xi\Sigma_s}(u'')\, du'' , \end{aligned}\right\} \tag{20}$$

Etc.

Neutron age is given by

$$d\tau = \frac{D\, du}{\xi\Sigma_s} , \qquad \tau(0) = 0 , \tag{21}$$

so that Eqs. (20) become:

$$G_0 = \left.\frac{1}{\xi\Sigma_s}\right|_\tau , \qquad G_1 = \left.\frac{1}{\xi\Sigma_s}\right|_\tau \tau , \qquad G_2 = \left.\frac{1}{\xi\Sigma_s}\right|_\tau \frac{\tau^2}{2} . \tag{22}$$

In general,

$$G_n = \left.\frac{1}{\xi\Sigma_s}\right|_\tau \frac{\tau^n}{n!} . \tag{23}$$

Further,

$$\int_0^\infty \nu\Sigma_f G_n \, du = k_\infty \left(\xi\Sigma_s G_n\right)_{\tau(U)} . \tag{24}$$

Therefore,

$$g_n = \frac{\tau(U)^n}{n!} \tag{25}$$

and

$$P(B) = \sum_0^\infty (-B^2)^n \frac{\tau(U)^n}{n!} = \exp\left\{-B^2\tau(U)\right\} . \tag{26}$$

This is, of course, the classical value.

A COMMENT ON THE G-SPECTRA OF FAST REACTORS

Typical fast reactors have essentially three spectral regions:

(1) At high energies, the spectrum is dominated by the interplay between the fission-spectrum source and inelastic scattering events involving large energy losses. Absorption is adequately represented by a smooth curve, both because of the extreme validity of the narrow resonance approximation and the smearing action of Doppler broadening on resonances.

(2) At intermediate energies, roughly 5-100 keV, the spectrum can be calculated quite well as a superposition of a gross spectrum, generated from continuous slowing-down theory with effective smeared absorption, and detailed resonance calculation.

(3) At lower energies, the continuous slowing-down model remains useful, but one must treat some resonances (such as those in sodium) in detail.

Most of the need for representation of the spectrum in many groups arises from the high-energy groups. In principle, continuous slowing-down should be adequate to describe energy transfer at the lower energies.

Now, if we note the trend of the G-spectra for the aging system, we observe that each G_{n+1} is <u>softer</u> than the previous G_n. We expect this to hold true for fast reactors as well. In essence, then, we may expect that, after the first few G_n, we can switch to a much simpler mathematical format to derive higher G_j; solution of the continuous slowing-down equations involves simple quadrature in u. Ultimately, the G_n should approach highly peaked functions which may be well approximated analytically.

THE ADJOINT FUNCTION

The same procedure as recommended for the flux may be used to determine an adjoint expansion.

The adjoint equation analogous to Eq. (5) is

$$\left[B_0^2 D(E) + \Sigma_a(E) + \Sigma_s(E)\right] S_0^+(E) - \Sigma_s(E) \int_0^E S_0^+(E') P(E \to E')\, dE'$$

$$= \nu\Sigma_f(E) \int_0^\infty \chi(E') S_0^+(E')\, dE' \,. \qquad (27)$$

For the infinite system, the adjoint spectrum is the solution of

$$\left[\Sigma_a(E) + \Sigma_s(E)\right] S_\infty^T(E) - \Sigma_s(E) \int_0^E S_0^+(E') P_s(E \to E')\, dE' = \nu\Sigma_f(E) \,. \qquad (28)$$

We may write a system of equations such that:

$$\left.\begin{aligned} G_0^+ &= S_\infty^+ \\ \left(\Sigma_a + \Sigma_s\right) G_{n+1}^+ - \Sigma_s \int_0^E G_{n+1}(E') P_s(E \to E')\, dE' &= D\, G_n \end{aligned}\right\} \,. \qquad (29)$$

Then we may write

Now, if we note the trend of the θ-spectra for the spike system, we observe that each θ^{n+1} is closer than the previous θ^n. We expect this to hold true for fast reactors as well. In essence, then, we may expect that, after the first few θ^n, we can switch to a much simpler mathematical format to derive higher ξ^n; solution of the continuous slowing-down equations involves single quadrature in u. Ultimately, the θ^n should approach highly peaked functions which may be well approximated analytically.

THE ADJOINT FRACTION

The same procedure as recommended for the flux may be used to determine an adjoint expansion.

The adjoint equation analogous to Eq. (3) is

$$\left[\Sigma_t^0(E) + \Sigma_c^0(E) + \Sigma_s^0(E)\right]\xi_+^0(E) - \Sigma_s^0(E)\int_0^\infty \xi_+^0(E')P_s^0(E' \to E)\,dE'$$

$$= \nu\Sigma_f^0(E)\int_0^\infty \chi(E')\xi_+^0(E')\,dE' \,. \qquad (27)$$

For the infinite system, the adjoint spectrum is the solution of

$$\left[\Sigma_t^0(E) + \Sigma_c^0(E)\right]\xi_\infty^0(E) - \Sigma_s^0(E)\int_0^\infty \xi_\infty^0(E')P_s^0(E' \to E)\,dE' = \nu\Sigma_f^0(E) \,. \qquad (28)$$

We may write a system of equations such that:

$$\begin{cases} \xi_+^0 = \xi_\infty^0 \\ \left[\Sigma_t^0 + \Sigma_c^0\right]\xi_+^{n+1} - \Sigma_s^0\int_0^\infty \xi_+^{n+1}(E')P_s^0(E' \to E)\,dE' = D\,\xi_+^n \end{cases} \qquad (29)$$

Then we may write

$$S_0^+ = \sum_0^\infty (-B_0^2)^n G_n^+ , \tag{30}$$

provided that

$$\int_0^\infty \chi(E') \sum_0^\infty (-B_0^2)^n G^+(E') \, dE' = 1 \tag{31}$$

is satisfied.

Let us multiply Eq. (28) by $G_0(E)$ — or $S_\infty(E)$ — and integrate over energy. This leads to the following equation after reversal of integration order and replacement of S_∞^+ by G_0^+:

$$\int_0^\infty G_0^+(E) \, dE \left[\Sigma_a + \Sigma_s\right] G_0 - \int_E^\infty \Sigma_s G_0(E') P_s(E' \to E) \, dE' = \int_0^\infty \nu\Sigma_f(E) G_0(E) \, dE . \tag{32}$$

Substituting Eq. (7) for the term in braces in Eq. (32),

$$\int_0^\infty G_0^+ \chi \, dE = \int \nu\Sigma_f G_0 \, dE = k_\infty . \tag{33}$$

We may thus define a critical condition

$$k_\infty P^+(B^2) = 1 , \tag{34}$$

where

$$P^+(B_0) = \sum_0^\infty (-B_0^2)^n g_n^+$$

$$g_n^+ = \int_0^\infty \chi(E) G_n^+ \, dE \int_0^\infty \chi(E) G_0^+ \, dE \tag{35}$$

It is well known that the buckling spectrum of flux and adjoint are identical. From this, it follows that

$$\left.\begin{aligned} P^{+}(B) &= P(B) \\ g_n^{+} &= g_n \ . \end{aligned}\right\} \qquad (36)$$

The adjoint function has the property of orthogonality to the real flux spectrum in the sense that:

If B_n^2 are the several values of B^2 which satisfy the critical equation [(17) or (34)]; and if

B_n^2 are all different.

Then

$$\int_0^\infty S_n(E)S_m^{+}(E)D(E)\,dE = 0 , \qquad \text{for } m \neq n , \qquad (37)$$

APPLICATION OF THE G-SPECTRA

The properties of the G spectra which can be applied stem from their (assumed) completeness and from the form of expansion of the fundamental mode. If the G_n are a complete set (which, except for pathological cases, they are), then they may perhaps be of use in defining alternate multigroup systems to the usual step-function-in-energy system. In particular, such a system might have the first group as fundamental mode, with other group spectra orthogonal to it. Then it would be possible to deal with transients, as introduced by reflectors and boundaries, more directly.

MULTIGROUP FORMULATIONS

In a multigroup model of standard type, $\phi(\vec{r},E)$ is replaced by an n-vector, $\vec{\phi}(\vec{r})$, where the "n" components of Φ represent the flux in

specified E-regions, D and Σ_a are diagonal matrices, integration over $\nu\Sigma_f$ is replaced by premultiplication by an n-adjoint-vector, $\chi(E)$ becomes a vector $\vec{X}$, and the scattering law is replaced by a transfer matrix.

The fundamental mode has a spectrum described by an eigenvector, and these are n-1 other eigenvectors which represent the higher-mode spectra. B_n^2 is often complex for $n > 0$, and the higher modes have complex spectra; however, n-1 linearly independent real spectra, all of which are orthogonal to the fundamental mode, can be synthesized from them.

The critical equation in an n-group system is always expressible in the form

$$k_\infty = \sum_{k=0}^{n} a_k B^{2k} . \tag{38}$$

This means that the criterion for good representation of any system by a multigroup scheme might by that 1/P(B) should be a series which terminates after a certain number of powers of B^2.

The most direct method of determining this is by formal inversion of P(B). We may write

$$1/P(B) = \sum_{k=0}^{\infty} a_k B^{2k} , \tag{39}$$

and derive the a_k iteratively from

$$\left.\begin{aligned} a_0 &= 1 \\ a_k &= \sum_{\ell=1}^{k} (-)^{\ell+1} a_{k-\ell} g_\ell \end{aligned}\right\} . \tag{40}$$

Because a_k and g_ℓ are dimensional, and because of cumulation of errors, it is recommended that convergence be examined by inspecting $a_{n+1}a_{n-1}/a_n^2$; if this number suddenly becomes small, an n-group approxi-

specified E-regions, U and Σ_a are diagonal matrices, integration over w_i is replaced by premultiplication by an n-adjoint-vector, $\chi(E)$ becomes a vector $\vec{\chi}$, and the scattering law is replaced by a transfer matrix.

The fundamental mode has a spectrum described by an eigenvector, and there are n-1 other eigenvectors which represent the higher-mode spectra. B_n^2 is often complex for $n > 0$, and the higher modes have complex spectra; however, n-1 linearly independent real spectra, all of which are orthogonal to the fundamental mode, can be synthesized from them.

The critical equation in an n-group system is always expressible in the form

$$k_\infty = \sum_{k=0}^{n} a_k B^{2k} , \qquad (38)$$

This means that the criterion for good representation of any system by a multigroup scheme might by that 1/P(B) should be a series which terminates after a certain number of powers of B^2.

The most direct method of determining this is by formal inversion of P(B). We may write

$$1/P(B) = \sum_{k=0}^{\infty} a_k B^{2k} , \qquad (39)$$

and derive the a_k iteratively from

$$\left\{ \begin{aligned} a_0 &= 1 \\ a_k &= \sum_{i=1}^{k} (-)^{i+1} a_{k-i} g_i \end{aligned} \right. \qquad (40)$$

Because a_k and g_k are dimensional, and because of cumulation of errors, it is recommended that convergence be examined by inspecting $a_{i+1}a_{n-1}/a_n^2$; if this number suddenly becomes small, an n-group approxi-

mation is justified. If, after many terms have been examined, there seems to be an approach to a constant ratio, an age-like solution can be suspected, and examination of the convergence of a_k to $\alpha T^k/k!$, where α and T are constants, is recommended.

If we have an N group system, G_N and higher will be linear combinations of $G_0, \ldots G_{N-1}$. Thus, all necessary relations can be obtained by computing 2N functions — N fluxes and adjoints, or 2N fluxes, which is algorithmically simpler.

Note that for a true N-group system, all a_n for $n > N$ must vanish. Thus, one should examine $a_{n+2}a_{n-2}/a_n^2$ etc., for a few terms before concluding that an N-group approximation is valid.

A mathematically more satisfactory way of determining the validity of an N-group approach is to determine the degree to which χ/D may be represented by a linear combination of $G_0 \ldots G_{N-1}$. If this is the case, G_{N-1} is a linear combination of χ/D and g's of lower order, whence G_N et seq. also are (from the recursion relations for G).

The equivalent statement is that G_N would likewise be a linear combination of $G_0 \ldots G_{N-1}$. A necessary condition for this to be the case is the vanishing of the determinant of g's to order 2N:

$$\begin{vmatrix} g_0 g_1 \cdots g_N \\ \cdot \quad \cdot \\ \cdot \quad \cdot \\ \cdot \quad \cdot \\ g_N \quad \cdots g_{2N} \end{vmatrix} = 0 .$$

This effectively states that there is a linear combination, P, of $G_0 \ldots G_{N-1}$ such that

$$\left.\begin{aligned} &\int_0^\infty G_m^+ D\left(G_N - P\right) dE = 0 \qquad m = 0, \ldots N-1 \\ &\text{and} \\ &\int_0^\infty \nu\Sigma_f\left(G_N - P\right) dE = 0 \,. \end{aligned}\right\} \tag{42}$$

It also means that $a_{n+1} \ldots a_{2N}$ all vanish. In other words, if the critical equation of form (39) has any terms of order greater than B^{2N}, they start at B^{4N+2}. While not mathematically impossible, such cases must be classified as pathological.

For comparison, the N-th order determinant for an age theory system would be of the order of:

$$\left(g_1\right)^{N^2+N}\left(\prod_0^N n!\right) \Big/ \left(\prod_N^{2N} n!\right) . \tag{43}$$

The determinant in Eq. (41) would have to be small compared to expression (43) in order to justify an N-group theory.

Once an N group theory has been established, we have some liberty in defining the groups which we shall use. All of them are, of course, linear combinations of the G_n.

The obvious choice is to define our groups orthogonal to each other, and to take as our first group the fundamental mode. To express it in terms of $G_0 \ldots G_{N-1}$ (remembering that G_N et seq. are themselves linear combinations of them), we start with the relation

$$g_{N+k} = -\sum_{\ell=1}^{N} (-)^\ell g_{N+k-\ell} a_\ell \,, \tag{44}$$

$$\begin{cases} \int_0^{\infty} s^m \left[(s^N - 1)^{-1} \right] ds = 0, & m = 0, \ldots, N-2 \\ \\ \int_0^{\infty} s^{N-1} \left[(s^N - 1)^{-1} \right] ds = \frac{\pi}{N} . \end{cases}$$

which follows from (40) and the vanishing of a_ℓ for $\ell > N$. It may now be shown that this corresponds to a similar expression for the G's:

$$\sum_{n=0}^{N} (-)^n a_n G_{n+k-n} = 0 , \qquad (k > 0) . \tag{45}$$

We now take Eq. (9), multiplying S_0 by k_∞ on the left-hand side and the infinite sum in Eq. (9) by the series expression for k_∞ in terms of B_0^2 [Eq. (38) with n = N). The use of Eq. (45) then leads to:

$$\left.\begin{aligned} S_0 &= \frac{1}{k_\infty} \sum_{n=0}^{N-1} (-)^n G_n \sum_{\ell=n}^{N-1} a_{\ell-n} B_0^{2\ell} \\ &= \frac{1}{k_\infty} \sum_{\ell=0}^{N-1} B_0^{2\ell} \sum_{n=0}^{\ell} (-)^n a_{\ell-n} G_n . \end{aligned}\right\} \tag{46}$$

Other groups may be defined to illustrate the transient spatial behavior of specific reactions. We may choose a group for one reaction which is orthogonal to the fundamental; a group for another which is orthogonal to the first two; and so on until we have N-2 reactions illustrated. Then the first reaction has a spatial dependence derived from the fundamental mode and the first of these synthetic groups; the spatial dependence of the second reaction depends on these two, plus the next synthetic group; and so on. (With the fundamental mode and N-2 such transients, we have a "ghost" group left over; at least one such "ghost" is needed in order to preserve group orthogonality.)

THE FISSION TRANSIENT

We illustrate the formation of groups by looking at a particularly straightforward one to synthesize. This is that transient which

incorporates all the fission rate which is not part of the fundamental mode. We look for a spectrum of the form $\alpha S_0 - \beta\chi/D = S_f$ which is orthogonal to S_0. Then, all other spectra which are linearly independent of S_0 and S_f will be orthogonal to them [in the $\int A^+(E)D(E)B(E)\,dE$ sense]. It follows that only S_0 and S_f will have nonvanishing integrals over $\nu\Sigma_f$.

If we now adopt the notation:

$$\langle AB \rangle \equiv \int_0^\infty A^+(E)D(E)B(E)\,dE\,, \tag{47}$$

the desired function is

$$\left\langle S_0 \frac{\chi}{D} \right\rangle S_0 - \langle S_0 S_0 \rangle \frac{\chi}{D} = S_f\,. \tag{48}$$

The representation of χ/D as a function of the G_n is now necessary. Formally, we may write

$$\frac{\chi}{D} = \sum_0^\infty X_n G_n \tag{49}$$

$$\gamma \equiv \left\langle \frac{\nu\Sigma_f}{D} \frac{\chi}{D} \right\rangle\,, \tag{50}$$

and obtain the x_n by solution of:

$$\begin{bmatrix} g_0, g_1, g_2, \cdots \\ g_1, g_2, g_3, \cdots \\ \cdot\ \cdot \\ \cdot\ \cdot\ \cdot \\ \cdot\ \cdot \\ \cdot\ \cdot \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_1 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} = \begin{bmatrix} \gamma \\ g_0 \\ g_1 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \tag{51}$$

Equation (51) is operationally difficult to solve, but conceptually

Note that the determinant of the matrix in Eq. (51) is, for a finite

approximation, the same one as is used to test the validity of a multigroup approximation of finite order.

THE MULTIGROUP EQUATIONS

We finish this first part of the specification of the method by seeing how we construct multigroup equations. Let us assume that we have completed the construction of S_0, S_f . . ., etc., in such a fashion that each one is orthogonal to the others. Let us further assume that we have, by hook or crook, arranged for the multigroup representation to be finite (this is a convenience rather than a necessity). Finally, let us label $S_0 \equiv Q_1$, $S_f = Q_2$ . . . up to Q_N. Thus, I have a set of

$$Q_i = \sum_{j=1}^{N} C_{ij} G_{j-1} , \tag{52}$$

where all the C_{ij} have been defined. Similarly,

$$Q_i^T = \sum_{j=1}^{N} C_{ij} G_{j-1}^{+} \tag{53}$$

and

$$\langle Q_i Q_j \rangle = 0 , \qquad i \neq j \tag{54}$$

We now write

$$\phi(\vec{r},E) = \sum_{k=1}^{N} Q_k(E) f_k(\vec{r}) , \tag{55}$$

and substitute into Eq. (2),

$$-\sum_{k=1}^{N} Q_k(E)D(E)\nabla^2 f_h(\vec{r}) + \sum_{k=1}^{N} f_k(\vec{r})\left\{\left[\Sigma_a(E) + \Sigma_s(E)\right]Q_k(E) - \int_E^\infty \Sigma_s(E')P_s(E' \to E)Q_k(E')\,dE'\right\}$$

$$= \chi(E)\sum_{k=1}^{N} f_k(\vec{r})\int_0^\infty \nu\Sigma_f(E')Q_k(E')\,dE' . \qquad (56)$$

Multiplying by Q_1^+ and integrating (remember, $Q_1 = S_0$) gives

$$-\left\langle Q_1Q_1\right\rangle\nabla^2 f_1 + \sum_{k=1}^{N} f_k(\vec{r})\left[\left\langle\frac{\nu\Sigma_f}{D}Q_k\right\rangle - D\,B_0^2\left\langle Q_1Q_1\right\rangle\right] = \sum_{k=1}^{N} f_k\left\langle\frac{\nu\Sigma_f}{D}Q_k\right\rangle , \qquad (57)$$

which reduces to

$$(\nabla^2 + B_0^2)f_1 = 0 ,$$

as it should.

Multiplication by Q_2^+ and integrating gives:

$$-\left\langle Q_2Q_2\right\rangle\nabla^2 f_2 + \sum f_k\lambda_{2k} = -\frac{\left\langle Q_2Q_2\right\rangle}{\left\langle Q_1Q_1\right\rangle}\left[f_1 - \frac{\left\langle Q_2Q_2\right\rangle}{\left\langle Q_1Q_1\right\rangle}f_2\right] . \qquad (58)$$

The λ_k are obtained by substituting the expansions for Q_n [into Eq. (52)] into Eq. (57), using the recursion relations for G_k, and substituting back the resulting expressions from G into Q.

Similar expressions are found by integrating over Q_n^+ for $n > 2$. The result is a set of N equations, of which the first, as fundamental mode,

is independent of the rest. The other N-1 equations represent a full matrix of equations with sources to the set coming from the fundamental mode. The Laplacian term is purely diagonal. The set is therefore determinate.

Each spectrum defines a D_k — an effective diffusion coefficient — such that $D_k \nabla f_k$ is continuous across normal boundaries. Also, each f_k is continuous (these properties derive from the detailed spectral continuities of the original equation). In general, it will prove impossible to satisfy all boundary conditions unless the reactor is critical.

REFLECTORS

Reflectors are, in general, nonmultiplying; therefore the χ terms will be small or vanish. Reflectors also have a different scattering maxtrix from cores, and different absorption.

The equations for the reflector must be obtained as in the core. It is assumed that the same set of orthogonal spectra describe the entire problem. Then the reflector equations become:

$$- \left\langle Q_k Q_k \right\rangle \nabla^2 f_{rk} + \sum_{k=1}^{N} f_{rk} \int_0^\infty \frac{D_c(E) Q_k}{D_r(E)} + dE \left[\Sigma_{a_r} + \Sigma_{s_r} - \int_E^\infty \Sigma_s Q_\ell P_s(E'' \to E)\, dE' \right]$$

$$= \int_0^\infty \chi \frac{D_c(E)}{D_r(E)} Q_k + (E) \sum_{\ell=1}^{N} f_{rk} \int_0^\infty \nu \Sigma_{fr} Q_\ell(E')\, dE' \,. \qquad (59)$$

The appropriate integrals must be evaluated to find a set of group equations for the f_{rk}.

FOOTNOTE

[a]A mathematically rigorous proof would require the demonstration that the G_n defined by Eqs. (10) and (12) form a complete set of functions in the space defined by solutions of Eq. (5). Our proof is equivalent to replacing the coefficient of χ in Eq. (5) by an arbitrary multiplier, assuming convergence of g_n, and identifying the multiplier as unity for a critical system. We think that it illustrates the physics better. Note also that we could have gotten to Eq. (4) directly by substituting Eqs. (9), (10), and (12) into Eq. (6).

REFERENCES

1. BEYER, F. C., et al., "The Fast Exponential Experiment," *Proc. Intern. Conf. Peaceful Uses of Atomic Energy, Geneva, 1958,* Vol. 5 (United Nations, New York), pp. 342-346.

2. CHEZEM, C. G., "A Uranium-Metal Exponential Experiment," *Nucl. Sci. Eng.*, 8, 652 (1960). This definitive paper cites most of the significant earlier work as well.

3. RAGO, A. L., and HUMMEL, H. H., "ELMOE: An IBM-704 Program Treating Elastic Scattering Resonances in Fast Reactors," Argonne National Laboratory Report ANL-6805 (1964). Needless to say the original ELMOE program has been translated to other machines and is now mostly available as a piece of other, larger programs.

4. BARBERGER, H., et al., "Analysis of Experiments Performed in MASURCA," in *Proc. Symp. on the Physics of Fast Reactor Operation and Design,* British Nuclear Energy Society (1969), pp. 25-39.

B